

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

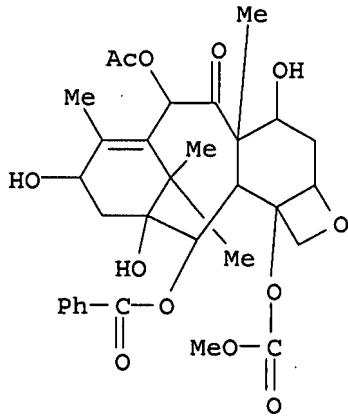
=> s 11 ful
FULL SEARCH INITIATED 18:01:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1419 TO ITERATE

100.0% PROCESSED 1419 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L2 6 SEA SSS FUL L1

=> d 1-6

L2 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN
RN 685564-38-9 REGISTRY
ED Entered STN: 25 May 2004
CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?,?-pentahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)
MF C31 H38 O14
CI IDS
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

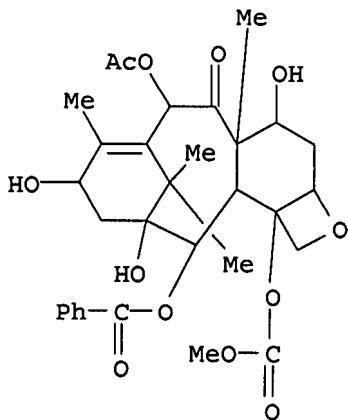


2 (D1-OH)

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 685564-30-1 REGISTRY
 ED Entered STN: 25 May 2004
 CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)
 MF C31 H38 O13
 CI IDS
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

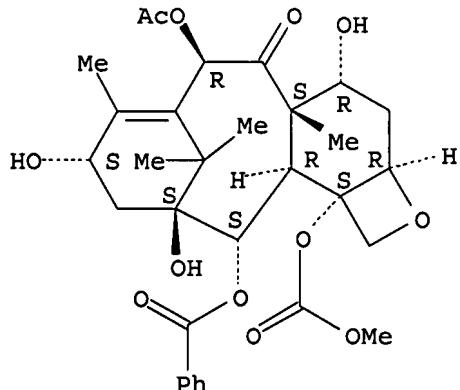


D1-OH

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 685096-39-3 REGISTRY
 ED Entered STN: 24 May 2004
 CN Carbonic acid, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C31 H38 O12
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

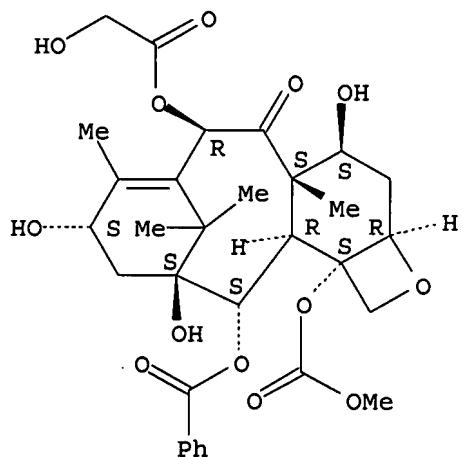


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 685096-38-2 REGISTRY
 ED Entered STN: 24 May 2004
 CN Acetic acid, hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C31 H38 O13
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

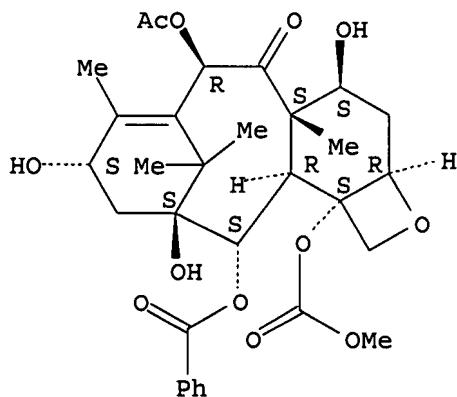


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 685096-28-0 REGISTRY
 ED Entered STN: 24 May 2004
 CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C31 H38 O12
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

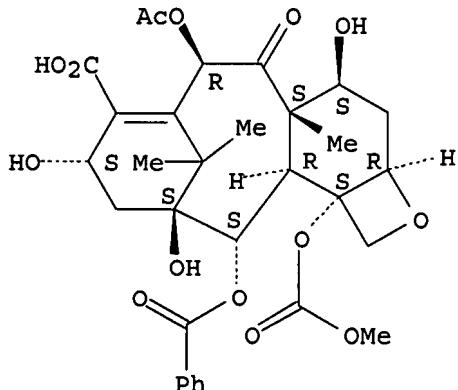


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 685096-27-9 REGISTRY
 ED Entered STN: 24 May 2004
 CN 7,11-Methano-1H-cyclodeca[3,4]benz[1,2-b]oxete-8-carboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,13,13-trimethyl-5-oxo-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C31 H36 O14
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

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	184.25	212.41
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.78

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 FILE LAST UPDATED: 6 May 2007 (20070506/ED)

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=> s 12
 L3 1 L2

=> d fbib abs hitstr

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:368898 CAPLUS
 DN 140:375336
 TI Characterization of taxane metabolites useful as tumor-growth inhibitors
 IN Comezoglu, S. Nilgun
 PA Bristol-Myers Squibb Company, USA
 SO PCT Int. Appl., 113 pp.
 CODEN: PIXXD2

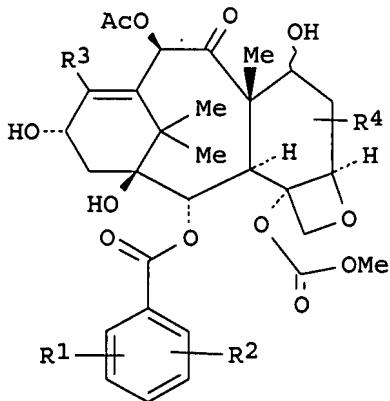
DT Patent

LA English

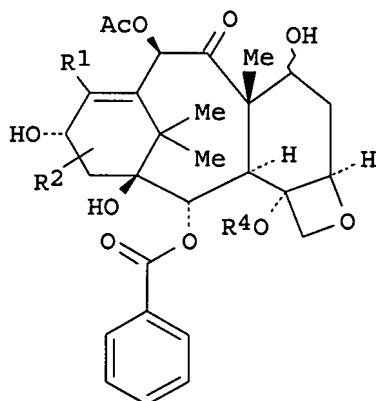
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004037211	A2	20040506	WO 2003-US34083	20031024
	WO 2004037211	A3	20040916		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003285005	A1	20040513	US 2002-421405P	P 20021025
				AU 2003-285005	20031024
				US 2002-421405P	P 20021025
				WO 2003-US34083	W 20031024
EP 1556030		A2	20050727	EP 2003-779320	20031024
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GI



I



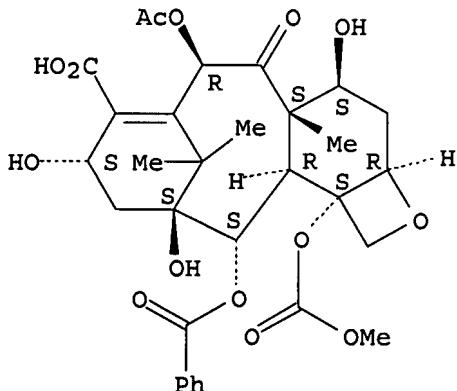
II

AB This invention relates to compds. that are metabolites of 3'-tert-butyl-3'-N-(tert-butyloxycarbonyl)-4-deacetyl-3'-dephenyl-3'-N-debenzoyl-4-O-(methoxycarbonyl)paclitaxel. The compds., e.g. I [R1 = SG,

OMe, OH, H, ; R2 = H, OH, OMe; R3 = Me, CO2H; R4 = H, OH, (OH)2; SG = SCH2CH(CONHCH2CO2H)NHC(O)CH2CH2CH(NH2)CO2H] and II [R1 = Me, CO2H; R2 = H, OH; R3 = COMe, H, COCH2OH; R4 = H, CO2Me], or a pharmaceutically acceptable salt, solvate or prodrug, are useful as therapeutic agents, especially as tumor-growth inhibitors. Thus, 14C-, 13C- and unlabeled 3'-tert-butyl-3'-N-(tert-butyloxycarbonyl)-4-deacetyl -3'-dephenyl-3'-N-debenzoyl-4-O-(methoxycarbonyl)paclitaxel were incubated with liver microsomes from various mammals and the metabolites were isolated and characterized.

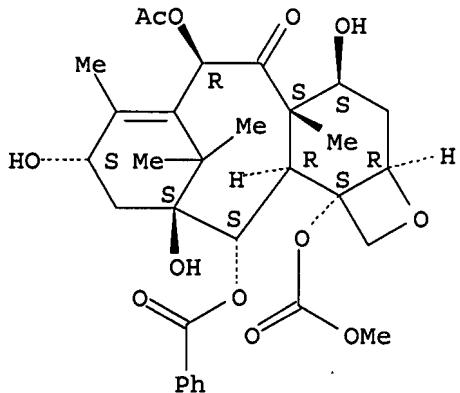
- IT 685096-27-9P 685096-28-0P 685096-38-2P
 685096-39-3P 685564-30-1DP, baccatin-ring hydroxyl regioisomers or epimer
 RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (characterization of taxane metabolites useful as tumor-growth inhibitors)
- RN 685096-27-9 CAPLUS
 CN 7,11-Methano-1H-cyclodeca[3,4]benz[1,2-b]oxete-8-carboxylic acid, 6-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,13,13-trimethyl-5-oxo-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- RN 685096-28-0 CAPLUS
 CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)

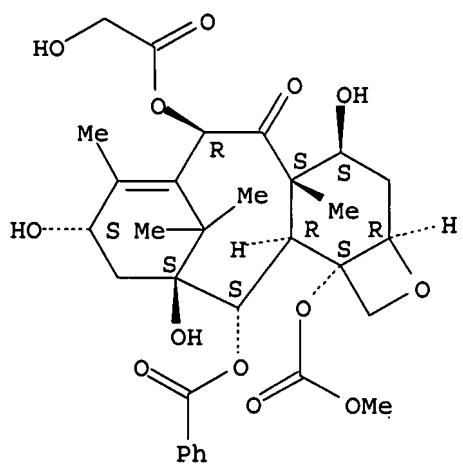
Absolute stereochemistry.



RN 685096-38-2 CAPLUS

CN Acetic acid, hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,9,11-trihydroxy-12b-[(methoxycarbonyl)oxy]-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)

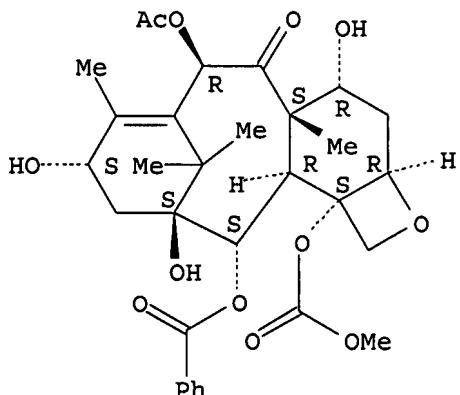
Absolute stereochemistry.



RN 685096-39-3 CAPLUS

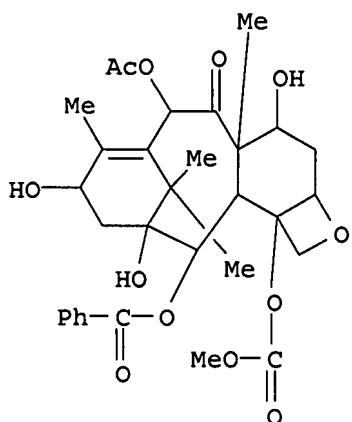
CN Carbonic acid, (2aR,4R,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 685564-30-1 CAPLUS

CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?-tetrahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)



D1-OH

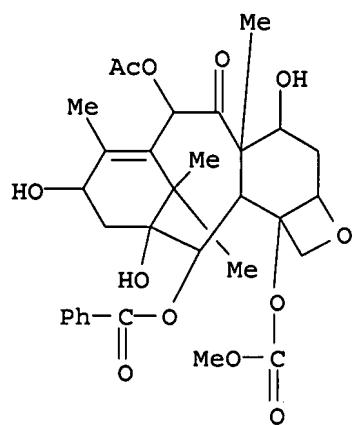
IT 685564-38-9P

RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

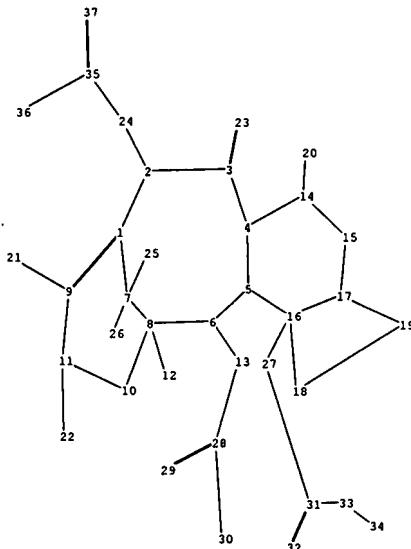
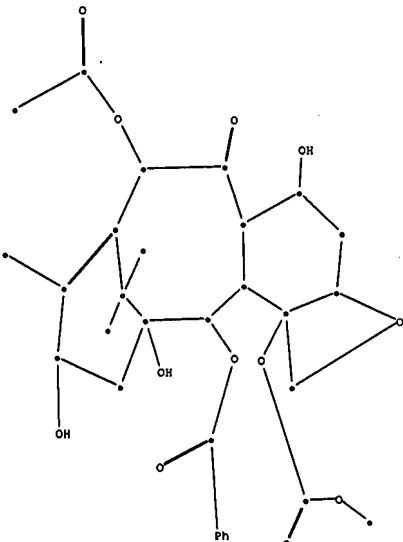
(incubation of, with mammal liver microsomes; characterization of taxane metabolites useful as tumor-growth inhibitors)

RN 685564-38-9 CAPLUS

CN Carbonic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6-(acetyloxy)-12-(benzoyloxy)-3,4,4a,5,6,9,10,11,12,12a-decahydro-4,9,11,?,?-pentahydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-12b(2aH)-yl methyl ester (9CI) (CA INDEX NAME)



2 (D1-OH)



chain nodes :

12 13 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18 19

chain bonds :

2-24 3-23 6-13 7-25 7-26 8-12 9-21 11-22 13-28 14-20 16-27 24-35 27-31 28-29 28-30
31-32 31-33 33-34 35-36 35-37

ring bonds :

1-2 1-7 1-9 2-3 3-4 4-5 4-14 5-6 5-16 6-8 7-8 8-10 9-11 10-11 14-15 15-17 16-17 16-18
17-19 18-19

exact/norm bonds :

1-2 1-7 1-9 2-3 2-24 3-4 3-23 4-5 4-14 5-6 5-16 6-8 6-13 7-8 8-10 8-12 9-11 10-11
11-22 13-28 14-15 14-20 15-17 16-17 16-18 16-27 17-19 18-19 24-35 27-31 28-29 31-32
31-33 33-34 35-37

exact bonds :

7-25 7-26 9-21 28-30 35-36

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:Atom 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS

10/5/2003

EAST - [space that works.wsp:1]

Search History

Grid Prefs... Font... Print Font: "Tahoma", Size: 10

Ref #	Hits	Search Query	DBS
L1	1133	((549/510) or (514/449)).CCLS.	USPAT
L2	364	I1 and paclitaxel	USPAT
L3	46	I2 and metabolite	USPAT
L4	46	I2 and metabolite	US-PGPUB; USPAT

Row Separation for Printout

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 Lines

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